

OPTIMIZATION METHODS FOR CHARACTERIZATION OF SINGLE PARTICLES FROM LIGHT SCATTERING PATTERNS

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ABSTRACT. We address the inverse light-scattering problem for particles described by a several-parameters model, when experimental data are given as an angle-resolved light-scattering pattern (LSP). This problem is reformulated as an optimization (nonlinear regression) problem, for which two solution methods are proposed. The first one is based on standard gradient optimization method, but with careful choice of the starting point. The second method is based on precalculated database of theoretical LSPs, from which the closest one to an experimental LSP is selected for characterization. We tested both methods for characterization of polystyrene microspheres using a scanning flow cytometer (SFC).

1. Introduction

The problem of single particle characterization from light scattering arises in different fields. An effective solution of this problem requires measuring LSPs, performed, e.g., by the SFC [1]. We assume that LSP can be computed for any particle, defining a map $f : X \rightarrow \mathbf{R}^d$, where $X \subset \mathbf{R}^p$ is a domain of particle parameters and $d \geq p$. The inverse problem consists in finding $f^{-1} : f(X) \rightarrow X$, which in most cases can be solved only numerically. The most general approach is optimization defined for any LSP (including noise) as

$$g : \mathbf{R}^d \rightarrow X, \quad g(y) = \arg \min_{x \in X} R_y(x), \quad R_y(x) = \|y - f(x)\|.$$

Robust optimization techniques are required due to oscillatory nature of the LSPs. In particular, stochastic global optimization techniques, multi-start Levenberg-Marquardt and DiRect methods were applied to single- and multi-layered spheres, e.g. [2, 3]. This comes at a great computational cost, which can be alleviated by using a preliminary exploration of the particular map f .

We propose two such methods. The “continuous” method is based on detailed analysis of the map f and its derivative, allowing one to rigorously construct a set of starting points $\{z_j\} \subset X$ such that for any $y = f(x)$ at least one of z_j would be a “good” starting point. The latter is defined so that the local minimization method starting from z_j will lead to x . The “discrete” method is based on a preliminary calculated database of theoretical LSPs and approximating g using the nearest-neighbor interpolation. This approach was used

previously, e.g. [4], but the issue of optimal structure and size of the database was not discussed. Here we propose an adaptive algorithm for database construction, which aims both at providing satisfactory local accuracy and at avoiding large errors of the inverse map. Details of these results can be found in [5, 6].

2. Optimization methods

To construct a set of starting points $\{z_j\}$ for the continuous method we start with a larger domain $X_1 \supset X$, and define several functions on X :

$$r(x) = \sup\{r > 0 \mid B(x, r) \subset X_1, \forall u \in B(x, r) \langle \nabla_u R_y(u), u - x \rangle > 0\},$$

where $y = f(x)$, $B(x, r)$ is the ball around x with radius r , and $\langle \cdot, \cdot \rangle$ denotes the inner product. The value $r(x)$ is the maximal radius such that gradient optimization starting at any point of the ball will lead to x . Let

$$t(x) = \inf_{u \in X_1 \setminus B(x, r(x))} R_y(u), \quad s(x) = \sup\{s > 0 \mid \forall u \in B(x, s) R_y(u) < t(x)\}.$$

The ball with radius $s(x)$ around global minimum x is deeper than any other local minima. The cover zone for any starting point z is

$$C(z) = \{x \in X \mid z \in B(x, s(x))\}.$$

A set of points $\{z_j\}$ is constructed iteratively until $X \subset \bigcup_j C(z_j)$. Then it can be proven that for any noise-free data $y \in f(X)$ starting point z_j with the minimum residual $R_y(z_j)$ is a good one.

The algorithm for database construction in the discrete method is the following. We use the same structure of the database as in DiRect method [3]. X is described by a set of hyperrectangles, whose centers constitute the database. New points are added to the database as a result of division of cells into three smaller hyperrectangles. We define $N(x)$ as a discrete set of neighbors in the database and fix the required accuracy ε . The database, set of pairs $(x, f(x))$, $x \in X_d$, is constructed iteratively until

$$\forall x \in X_d \quad \forall u \in N(x) \quad \forall v \in X_d \setminus B(x, \varepsilon) \quad \|f(u) - f(x)\| < \|f(v) - f(x)\|.$$

First, this condition implies that $\forall x \in X_d \quad N(x) \subset B(x, \varepsilon)$, i.e. the database is sufficiently locally dense. Second, it aims to sufficiently discretize those parts of X that may lead to large errors of approximation of the map g .

3. Results for spheres

Both methods were applied for characterization of homogeneous spheres using the LSPs measured by the SFC [1]

$$I(\theta) = \frac{w(\theta)}{2\pi} \int_0^{2\pi} d\varphi [S_{11}(\theta, \varphi) + S_{14}(\theta, \varphi)], \quad w(\theta) = \frac{1^\circ}{\theta} \exp(-2 \ln^2(\theta/54^\circ))$$

in the range of $\theta \in [10^\circ, 70^\circ]$. The initial domain X for size parameter α and relative refractive index m was chosen as $[5, 40] \times [1.05, 1.3]$. The number of starting points for the continuous method were 2458, while the number of LSPs in the database for the discrete method were 9366.

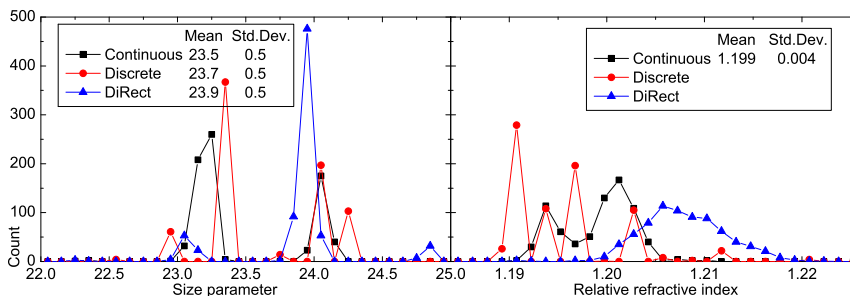


Figure 1. Distributions of a sample of polystyrene microspheres over α and m , obtained by processing LSPs measured with a SFC by proposed methods in comparison with reference DiRect method.

First, the methods were tested on synthetic data covering the whole X resulting in good accuracy. Moreover, the methods proved resistant both to white noise (up to 20% amplitude) and to shape distortions of the synthetic particles (spheres were replaced by spheroids with aspect ratios between 0.9 and 1.1). Second, we applied both methods to real experimental data for polystyrene microspheres in the buffer solution with refractive index 1.337. According to the producer's data, mean α of microspheres is 25 with coefficient of variation 4%. Relative refractive index of bulk polystyrene at this wavelength is 1.185. Here we present the results only for experimental data—see figure 1. Typical computational time to process one spherical particle on a 2.3 GHz processor is 0.02 s for both proposed methods and 1.6 s for the DiRect.

4. Conclusion

We proposed two methods to characterize particles from LSPs. The continuous method is better suited for shapes that permit quick simulation of LSPs, e.g. multi-layered spheres. On contrary, the discrete method is preferable for non-spherical particles. They were tested on synthetic and experimental data for spheres. However, we are currently working on their application to more interesting cases, such as lymphocytes and erythrocytes. We will present our first results in this direction at the conference.

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